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Title: High Fidelity Tomographic Density Reconstructions

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High Fidelity Tomographic Density Reconstructions

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Jennie Schei Disterhaupt (J-4), Michael McCann (T-5)

Technology Demonstration
October 10/2021

High Fidelity Tomographic Density Reconstructions

Background

Pressed high explosives have small density variations associated with the pressing process, from a few to sub percent depending on the material . [1] Variations at these levels are known to have an impact on HE performance [2] Currently, a destructive testing method based on physical sectioning followed by immersion density measurements (slice and dice) is utilized. However, this method has poor spatial resolution limited by the the sectioning size, 1-2 cm. [2] If possible, radiographic methods including Computed Tomography (CT) would be preferred, as they are non-destructive and have higher (less than .1 mm) spatial resolution. However, beam hardening, scattered radiation, and detector effects make density reconstructions at this level extremely challenging.

Proposed Work

The quantitative determination of small density variations within a volume using CT presents a challenge utilizing existing reconstruction algorithms. Recently, we have develop a number of enabling algorithms to address this problem. To validation of these tomographic density reconstructions requires the design of experiments and subsequent tomographic analysis. In this work we have designed and performed experiments to allow for the application of these techniques to enable the application of these algorithms to improving quantitative density reconstructions.

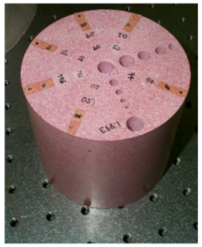
1. L. Hill and T. Salyer, "The los alamos enhanced corner-turning (ecot) test," in Proceedings of the 16th International

Detonation Symposium, (2018).

2. N. Stull, M. Espy, L. Hill, A. Figueroa, C. Gautier, J. Hunter, S. Larson, B. Olinger, and D. Thompson, "Finding small density gradients in high explosives non-destructively using x-ray computed tomography," in AIP Conference Proceedings, , vol. 2272 (AIP Publishing LLC, 2020), p. 060035

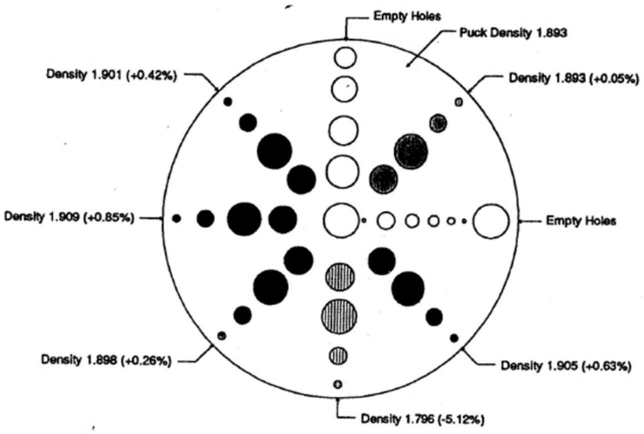
3. M. L. Klasky, B. T. Nadiga, J. L. S. Disterhaupt, E. Guardincerri, J. L. Carroll, L. A. Pfister, L. D. Hovey, E. W. Skau, G. P. Salazar, B. J. Warthen et al., "Hydrodynamic and radiographic toolbox (hart)," Tech. rep., Los Alamos National Lab.(LANL), Los Alamos, NM (United States) (2020).

Objective Continued



What do we think we could see?

- Pink Mock with calibrated inserts
- Best case modeling from Viskoe and Dohohoe* indicates that 0.26% are theoretically visible
- To date we have not measured to better than the 5% variation on this phantom

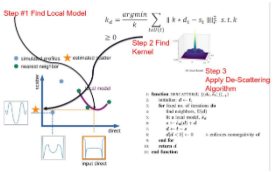


* IEEE Trans. Inst. and Meas. 45(1) Feb. 1996

Enabling Technologies

Local Kernel Based De-Scattering

- **Method of treating scattered radiation to enable density reconstructions developed via work for the Defense Threat Reduction Agency (DTRA)**



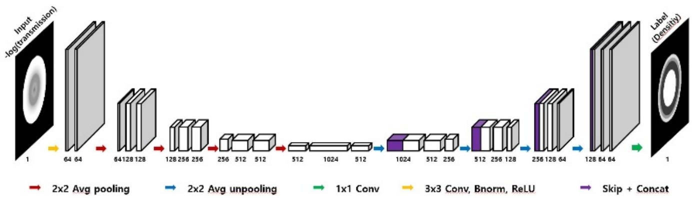
Approach can estimate and remove scatter very quickly

McCann, Klasky et. al Local Models for Scatter Estimation and Descattering in Polyenergetic X Ray Tomography, Optics Express (In Press)

Radiographic Inversion using Machine Learning

- **Method to invert radiographic, de-scattered image, using Convolutional Neural Network developed via work for the Defense Threat Reduction Agency (DTRA)**

Network Architecture: **Hourglass structure**



Detector Modeling

Transport calculations and experimental validation to detector modeling developed via work for the Defense Threat Reduction Agency (DTRA)

Enabling Technologies (Continued)

- **Framework for inclusion of priors into inverse problems (SCICO) developed under LDRD**

Few-view CT Example

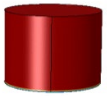
$$\min_x \frac{1}{2}\|y - Ax\|_2^2 + \lambda\|Cx\|_1$$

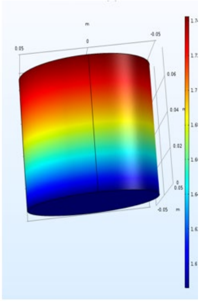
```
# Set up the problem
A = scico.linop.ParallelProjector(config)
L = scico.losses.SquaredL2Norm(y, A)
f = lambda_ * scico.functionals.SquaredL2Norm()
C = scico.linop.FiniteDifference2D()
admm = scico.admm.ADMM(L, f_list=[f], C_list=[C])

# Execute!
admm.init()
admm.run()
```

- `ParallelProjector` calls `ASTRA` GPU-based Radon transform
- Reconstruction of 1024×1024 area from 100 views in $\approx$ 1 minute

- **Finite Element modeling for validation experiments using COMSOL**

Comsol allows for
parametric examination of
Changes in density, thermal conductivity, and coefficient of thermal expansion to build database of simulations for machine learning prior.



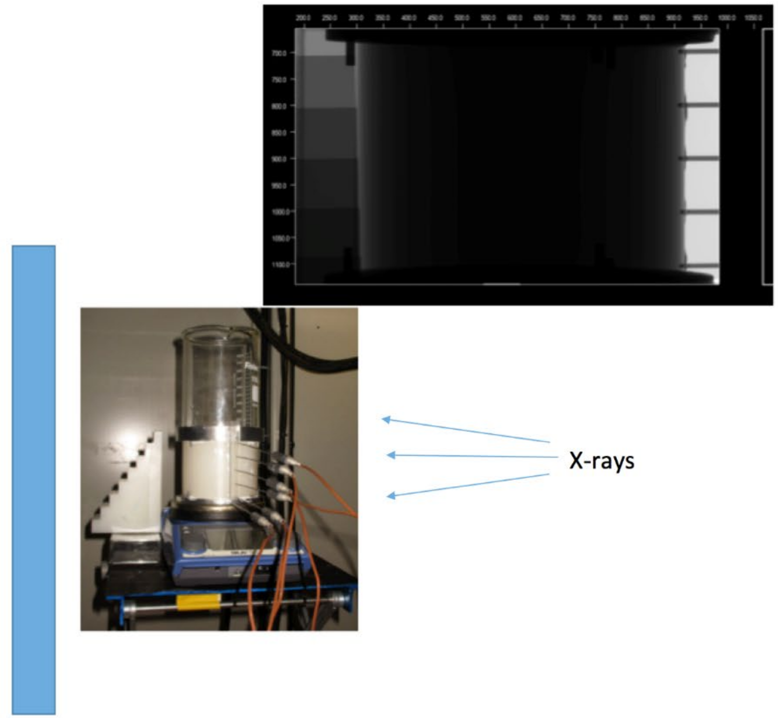


- **Micro CT Facilities E-6**

Experimental design of validation experiments

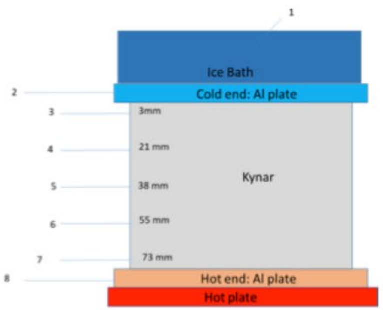
Experimental design of heated cylinder experiments were performed in an attempt simplify experimental conditions for heat transfer modeling and reduce experimental uncertainties.

Radiograph



Detector

- Kynar Cylinder
- Kynar step-wedge



Development of prior from Finite Element Modeling and Mathematical Analysis

- **An ensemble of simulations were developed for the experimental configurations by varying both the thermal properties of the cylinder as well as the heat transfer coefficient from the slides.**
- **These simulations were utilized to build a thermal model manifold using the variations of parameters:**

Thermal properties of Kynar

W.N. dos Santos et al. / Polymer Testing 27 (2008) 204–208

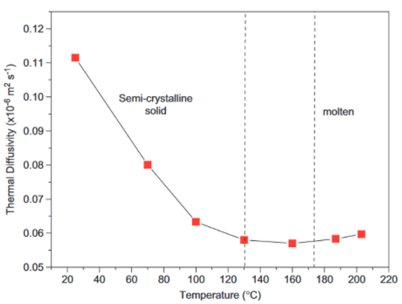


Fig. 1. Thermal diffusivity as a function of temperature.

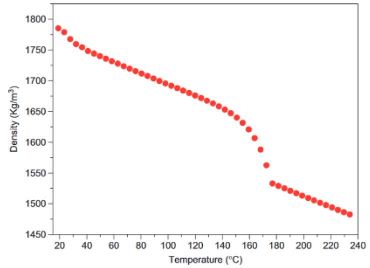


Fig. 3. Density as a function of temperature.

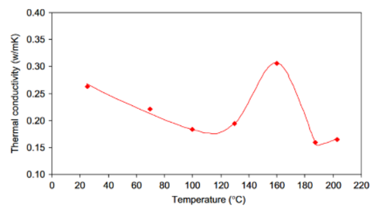


Fig. 4. Thermal conductivity of PVDF as a function of temperature.

Heat transfer coefficient varied from 0 to XX

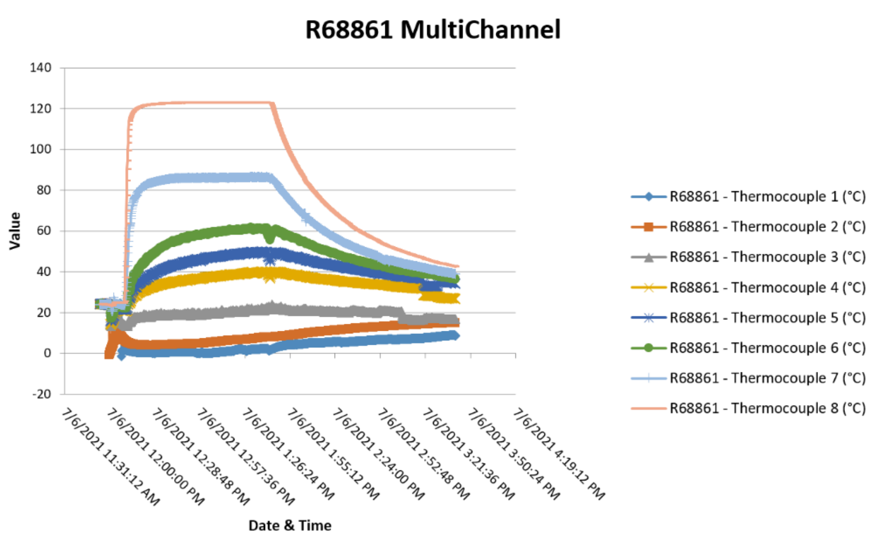
Radiographic Training database for heated cylinder validation experiment & detector developed

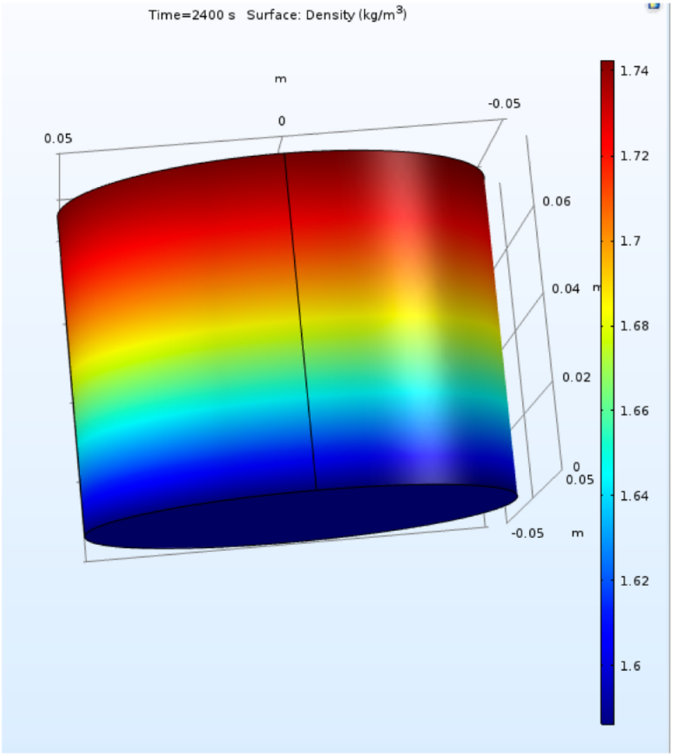
- To enable the reconstruction algorithm we have generated a dataset consisting of 2500 cylindrically symmetric HE density objects and calculated the corresponding direct, scattered radiation, and accompanying energy spectra using MCNP6 [5]. Detector response of the Perkin Elmer 1621 flat panel was also incorporated into the forward modeling for use in the de-scattering and CNN training.

- The objects consisted of cylinders with a fixed outer radius with variable density profiles in both the radial and azimuth direction.

Experimental Temperature Measurements and Heat Transfer Simulations

Thermal modeling

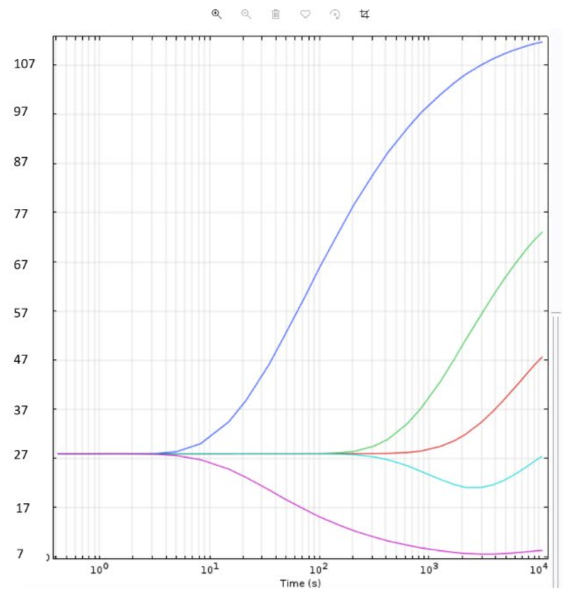


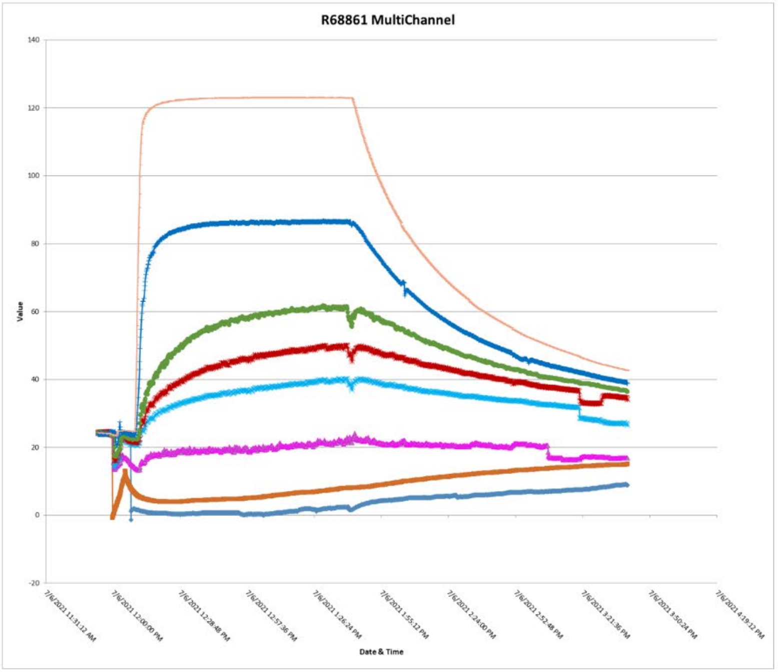


At ~12:00 hot plate turned on and ice applied; at ~13:40 hot plate turned off

Thermal Modeling of Baseline Experiment and Experimental results

Thermal model vs data

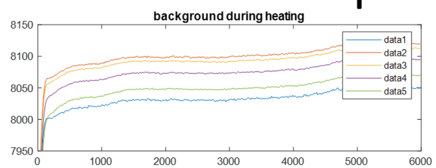


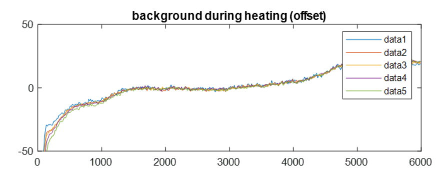


- Agreement isn't great… but conditions quite different

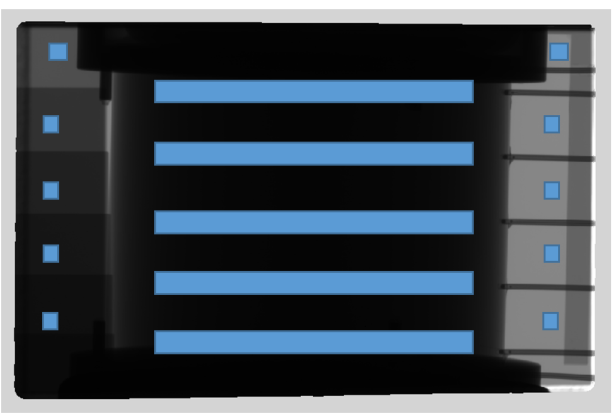
Radiographic correlations in heated cylinder experiments

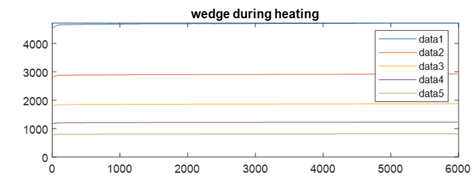
Trends in the part: heating

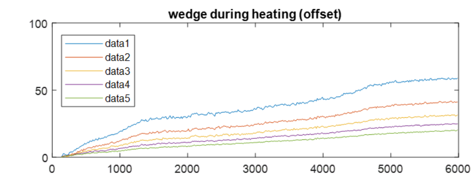




These overlay after adjusting for offset – which seems reassuring

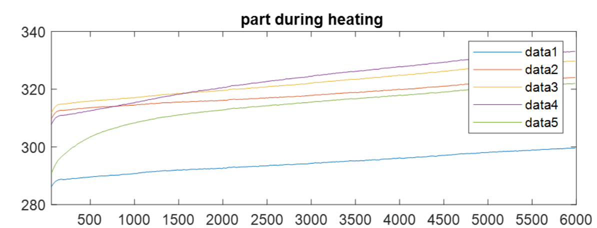


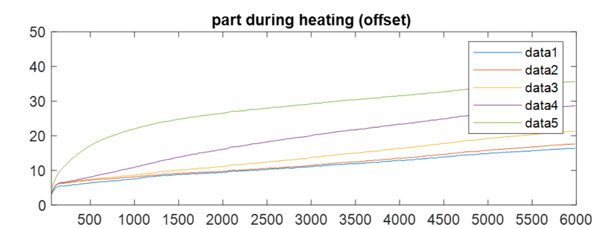




Why don't these overlay?

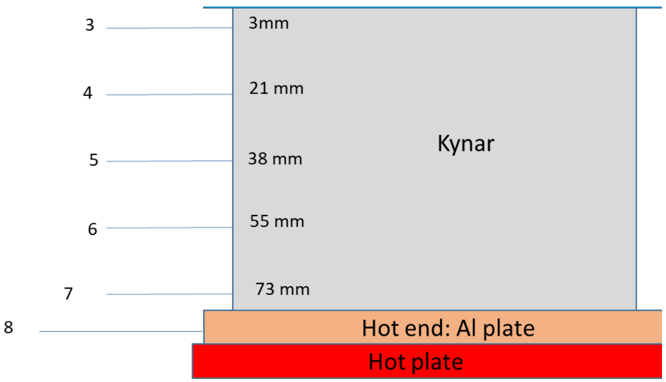
Using ratios of counts we get
1.62
1.56
1.53
1.51
?



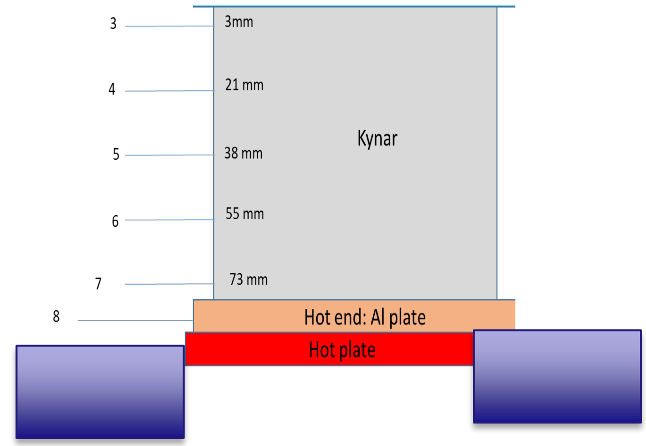


Modifications of Experiments

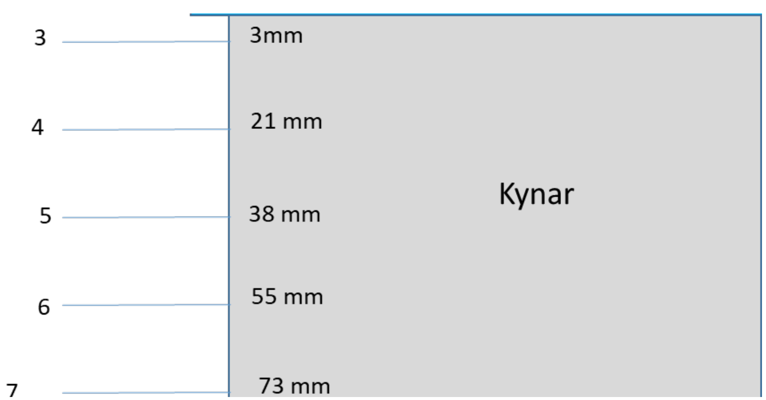
- **Analysis of experimental results from baseline experiment led to several experimental design changes including:**
  - Removal of Ice Bath (cooling)
  - Use of Insulation to shield thermo-couples from heat source
  - Preheating the cylinder



Insulation of Thermo-Couples



Removal of Ice Bath

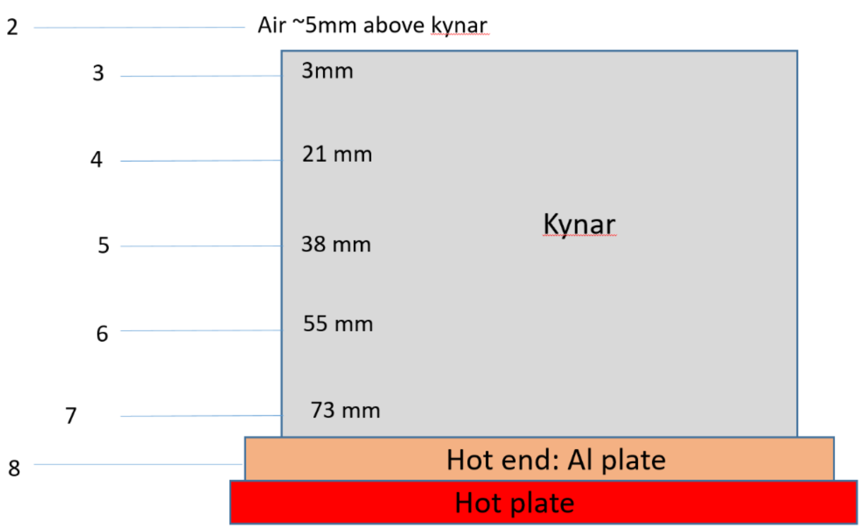


Preheated Cylinder

Experimental modification I

Based on the examination of the experimental measurements to the heat conduction simulations it was concluded that the ice bath was not performing cooling as anticipated i.e. the B.C. on the cool side was not maintained. Consequently, the ice bath was removed to provide a convective boundary condition.

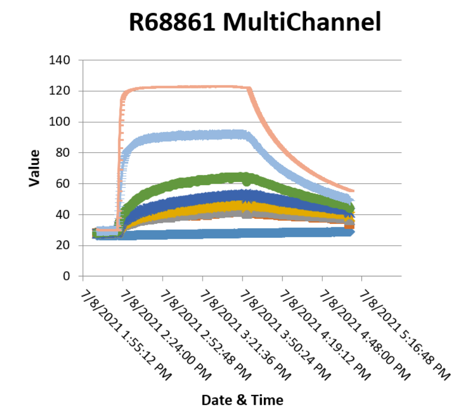
- Only one end of the part is heated – the other open to air

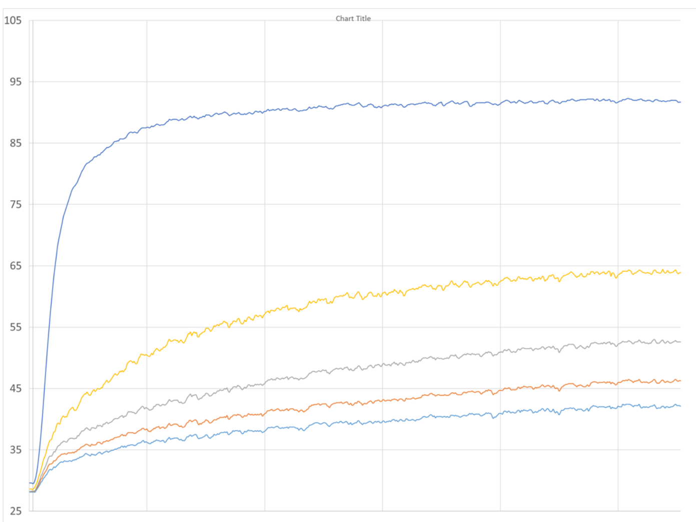


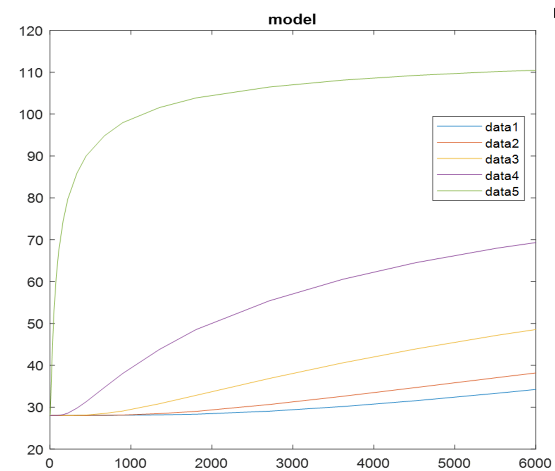
Comparison of Simulated Heat Transfer and the Experimental Results

Thermocouples vs. model

- Again we see the lack of lag in thermocouple data



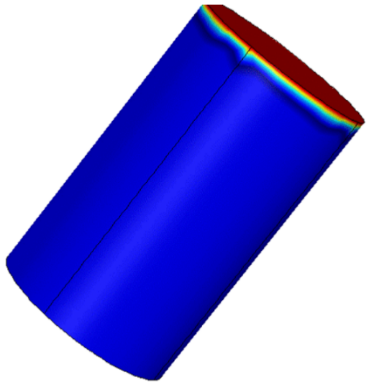




Summary of Work

The thermal gradient was 3-5% at maximum

- We could tell differences at intermediate points so at the 1% level
- This should be adequate to tell gradients in 9502 (but not 9501)
- 100 pixels = 18 mm in the image
- Effective pixel is .18mm
- Panel was 2x2 (effective pixel .127x2) = 0.254
- Mag was ~1.41
- Part should expand ~ 0.8mm or 5 pixels
- That is what we observed



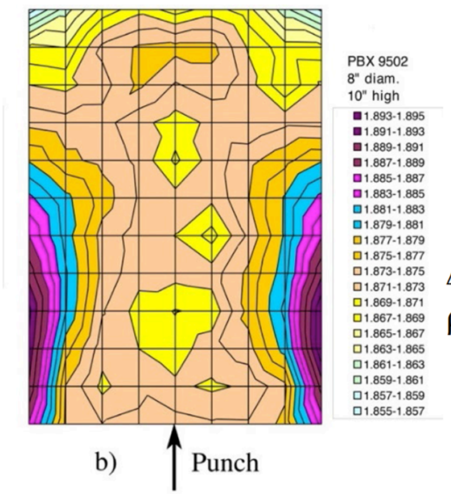
Program Impact

- We have showed progress in the application of our tomographic reconstruction algorithms. The prior comparisons with the data have led to modifications of the experimental design.
- Examination of the radiographic data also suggest that density inversion may lead to observable density gradients.
- Progress has been documented via a Optical Society Paper , Vancouver, Canada July 2021
- Impact has been reflected in FY 22 Funding from the Life Time and Aging Program and potential funding from the Emergency Response Program (Proposal Submitted to DTRA)

It is hard to measure very small changes in density

- The state-of-the art for measuring density to 0.1% in pressed cylinders of HE is destructive "slice and dice" method by Bart Olinger

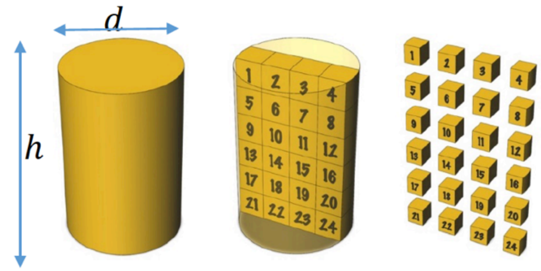
  - 13 cylinders of PBX 9502
  - 1" cubes (in all but one case); various aspect ratios (AR)
  - Slice-and-dice uncertainty principle: accurately specify density (large samples), or position (small samples), but not both @ same time.



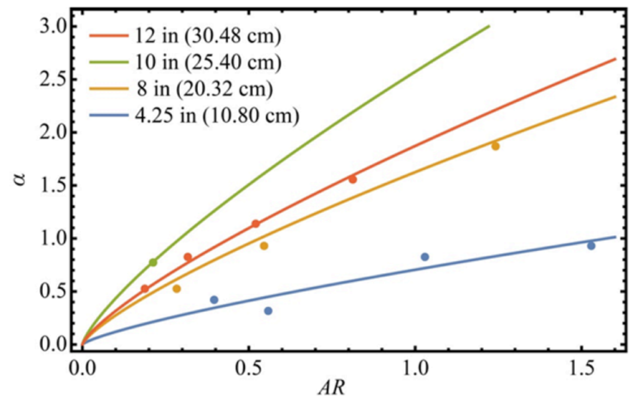
$\Delta\rho$=.075g/cc

ρ_{tmd} = 1.942 g/cc.

$$\alpha = \frac{\Delta\rho}{\rho_{tmd}} \cdot 100$$



$$AR = h/d$$



Dependence of α on AR, for four fixed d-values in 9502

CT would be a good method but measuring density changes at sub-percent is challenging

- CT involves taking numerous radiographs over 360°
- Attenuation depends on Beer-Lambert $I=I_0\exp(-\mu x)$
- μ is attenuation coefficient that depends on material and beam energy (*hv*)
- Our source is not mono-energetic

✓Beam hardening

✓Scatter

✓ (we'll get back to these)

$$\mu \sim k\frac{p}{A}\frac{Z^4}{(hv)^3}$$

$$mag = \frac{L1 + L2}{L1}$$